

Elastic Fields of Dislocations in Anisotropic Media

— a talk given at the group meeting

Jie Yin, David M. Barnett and Wei Cai

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1 Why I want to give this talk

- Show interesting features on the physics and math of dislocations.
- I am impressed by the ingenious way of solving the very complex PDEs, e.g. $C_{ijkl} u_{k,li} = 0$.

2 Outline

1. Short review of linear elasticity (general, 3-D)
2. Setup of anisotropic elasticity equations in 2-D
3. Solve for the elastic field of an infinite dislocation line
4. Express the stress field of a dislocation segment (next talk)

3 Short Review of Linear Elasticity

3.1 Displacement

Point \mathbf{X} moves to \mathbf{x} when the continuum media is deformed. The displacement is defined as

$$\mathbf{u} = \mathbf{x} - \mathbf{X} \quad \text{or} \quad u_i = x_i - X_i \quad (i = 1, 2, 3) \quad (1)$$

When the deformation is infinitesimal, we can ignore the difference between \mathbf{X} and \mathbf{x} . Thus

$$\mathbf{u}(\mathbf{x}) = \mathbf{u}(\mathbf{X} + \mathbf{u}) \approx \mathbf{u}(\mathbf{X}) \quad (2)$$

3.2 Strain

Strain field, ϵ_{ij} is defined as following,

$$\epsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i}) \quad (3)$$

where $u_{i,j} = \partial u_i / \partial x_j$, therefore $\epsilon_{ij} = \epsilon_{ji}$ (symmetry). When \mathbf{x} is three-dimensional vector, $u_i(\mathbf{x})$ has only 3 degrees of freedom(DoF), while $\epsilon_{ij}(\mathbf{x})$ has 6. Since strains are defined by displacements, there must be some relation between the components of ϵ_{ij} , i.e. **compatibility condition**,

$$\epsilon_{ij,kl} + \epsilon_{kl,ij} - \epsilon_{ik,jl} - \epsilon_{jl,ik} = 0 \quad (4)$$

When solving elasticity problems, if the final equations are written in terms of $u_i(\mathbf{x})$, we don't need to apply this condition. However, when final equations involve ϵ_{ij} or σ_{ij} , compatibility condition becomes essential for final solutions.

3.3 Stress

Stress field, σ_{ij} is defined by **Generalized Hooke's Law**

$$\sigma_{ij} = C_{ijkl}\epsilon_{kl} \quad (5)$$

C_{ijkl} is elastic stiffness (or constant) tensor, related to the mechanical properties of materials. Since both ϵ_{ij} and σ_{ij} are symmetric, C_{ijkl} satisfies following symmetries,

$$C_{ijkl} = C_{jikl} = C_{klij} = C_{klji} \quad (6)$$

therefore it has only 21 independent components.

For cubic crystals,

$$C_{ijkl} = C_{44}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) + C_{12}\delta_{ij}\delta_{kl} - H\delta_{ij}\delta_{kl}\delta_{ik} \quad (7)$$

where $H = 2C_{44} + C_{12} - C_{11}$, C_{11} , C_{12} and C_{44} are three independent elastic constants. A cubic crystal becomes elastically isotropic when $H = 0$.

For isotropic materials,

$$C_{ijkl} = \lambda\delta_{ij}\delta_{kl} + \mu(\delta_{ij}\delta_{kl} + \delta_{il}\delta_{jk}) \quad (8)$$

thus stress expression can be simplified as

$$\sigma_{ij} = \lambda\epsilon_{kk}\delta_{ij} + 2\mu\epsilon_{ij} \quad (9)$$

3.4 Equilibrium Condition

The governing equation of motion is

$$\sigma_{ij,i} + b_j = \rho\frac{\partial^2 u_j}{\partial t^2} \quad (10)$$

where \mathbf{b} is the body force and ρ is the mass density.

At equilibrium, $\partial^2 u_j / \partial t^2 = 0$, using Hooke's Law, Eq. (5), we have

$$C_{ijkl} u_{k,il} + b_j = 0 \quad (11)$$

Solution to steady-state problems in linear elasticity is equivalent to solving the above equation together with associated boundary and initial conditions for the displacement field \mathbf{u} .

4 Equations for an Infinite Dislocation Line

For an anisotropic medium whose elastic stiffness constants C_{ijkl} are relative to the $\mathbf{e}_1 - \mathbf{e}_2 - \mathbf{e}_3$ natural crystal basis, \mathbf{x} denotes a position from origin \mathbf{O} , a mutually orthogonal right hand basis $\mathbf{m}-\mathbf{n}-\mathbf{t}$ has been chose to solve the problem. Thus

$$\mathbf{x} = (\mathbf{m} \cdot \mathbf{x}, \mathbf{n} \cdot \mathbf{x}, \mathbf{t} \cdot \mathbf{x})^T \quad (12)$$

Assuming

1. $b_j = 0$, i.e. there is no body force;
2. the solution of \mathbf{u} is independent of x_3 , i.e. invariant along the dislocation line;

Stroh suggested a displacement field of the form,

$$u_k = A_k f(m \cdot x + p n \cdot x) \quad (13)$$

where \mathbf{A} is a constant vector, p is a constant and f is an arbitrary analytical function. Plugging this trial solution into Eq. (11) gives,

$$\{C_{ijkl}(m_i + p n_i)(m_l + p n_l)\} f'' A_k = 0 \quad (14)$$

Consider the case $f'' = 0$, it gives a solution of constant strain field, which is impossible for dislocations. thus

$$\{C_{ijkl}(m_i + p n_i)(m_l + p n_l)\} A_k = 0 \quad (15)$$

A nontrivial solution for \mathbf{A} exists only if

$$\|C_{ijkl}(m_i + p n_i)(m_l + p n_l)\| = 0 \quad (16)$$

where $\| \cdot \|$ stands for the determinant. It is a sixth-degree polynomial (with real coefficients) equation in p . The general solution to the displacement field can be written as a linear combination of the six solutions corresponding to p_α , i.e.,

$$u_k = \sum_{\alpha=1}^6 D_\alpha A_{k\alpha} f(\mathbf{m} \cdot \mathbf{x} + p_\alpha \mathbf{n} \cdot \mathbf{x}) \quad (17)$$

where D_α are coefficients determined by the boundary conditions of the elastic problem under consideration. To sum up, solving p enables solving \mathbf{A} , coefficient D_α are dependent on p_α and B.C. (General PDE strategy)

5 Solve for the Elastic Field of Infinite Dislocation Line

To solve the above problem, several approaches exist, including the **Matrix Formalism** and the **Integral Formalism**. Here I will focus on the Matrix Formalism.

5.1 Solve for \mathbf{p} and \mathbf{A}

Eq. (18) can be rewritten as

$$C_{ijkl}(m_i + p_\alpha n_i)(m_l + p_\alpha n_l) A_{k\alpha} = 0 \quad (18)$$

The basic idea is to convert Eq. (18) into an eigenvalue problem, which is easier to solve than the polynomial. A new variant, vector \mathbf{L} is introduced,

$$L_{j\alpha} = -n_i C_{ijkl}(m_l + p_\alpha n_l) A_{k\alpha} \quad (19)$$

Alternatively, by expanding Eq. (18), we have

$$L_{j\alpha} = \frac{1}{p_\alpha} m_i C_{ijkl}(m_l + p_\alpha n_l) A_{k\alpha} \quad (20)$$

We render $A_{k\alpha}$ and $L_{k\alpha}$ unique by the normalization condition

$$2A_{k\alpha} L_{k\alpha} = 1 \quad (\text{no sum on } \alpha) \quad (21)$$

Using following notation

$$(ab)_{jk} = a_i C_{ijkl} b_l \quad (22)$$

we may rewrite Eq. (19) and Eq. (20) as

$$(nm)_{jk} A_{k\alpha} + L_{j\alpha} = -p_\alpha (nn)_{jk} A_{k\alpha} \quad (23)$$

$$(mm)_{jk} A_{k\alpha} = -p_\alpha (mn)_{jk} A_{k\alpha} + p_\alpha L_{j\alpha} \quad (24)$$

In terms of six-dimensional matrices, it becomes

$$\begin{Bmatrix} (nm) & I \\ (mm) & O \end{Bmatrix} \begin{Bmatrix} \mathbf{A}_\alpha \\ \mathbf{L}_\alpha \end{Bmatrix} = p_\alpha \begin{Bmatrix} -(nn) & O \\ -(mn) & I \end{Bmatrix} \begin{Bmatrix} \mathbf{A}_\alpha \\ \mathbf{L}_\alpha \end{Bmatrix} \quad (25)$$

where

$$\begin{Bmatrix} \mathbf{A}_\alpha \\ \mathbf{L}_\alpha \end{Bmatrix} = \begin{Bmatrix} A_{k\alpha} \\ L_{k\alpha} \end{Bmatrix} = \begin{Bmatrix} A_{1\alpha} \\ A_{2\alpha} \\ A_{3\alpha} \\ L_{1\alpha} \\ L_{2\alpha} \\ L_{3\alpha} \end{Bmatrix} \quad (26)$$

Multiply both sides of Eq. (25) (from left) by

$$-\begin{Bmatrix} -(nn)^{-1} & O \\ -(mn)(nn)^{-1} & -I \end{Bmatrix}$$

and noting that

$$-\begin{Bmatrix} -(nn)^{-1} & O \\ -(mn)(nn)^{-1} & -I \end{Bmatrix} \begin{Bmatrix} -(nn) & O \\ -(mn) & I \end{Bmatrix} = \begin{Bmatrix} I & O \\ O & I \end{Bmatrix} \quad (27)$$

we obtain the following eigen equation,

$$\mathbf{N}\xi_\alpha = p_\alpha\xi_\alpha \quad (28)$$

where

$$\mathbf{N} = -\begin{bmatrix} (nn)^{-1}(nm) & (nn)^{-1} \\ (mn)(nn)^{-1}(nm) - (mm) & (mn)(nn)^{-1} \end{bmatrix} \quad (29)$$

$$\xi_\alpha = \begin{pmatrix} A_\alpha \\ L_\alpha \end{pmatrix} \quad (30)$$

Here is a convention for the the subscript α 's

$$\begin{aligned} \text{Im}(p_\alpha) > 0 & \quad \alpha = 1, 2, 3 \\ \text{Im}(p_\alpha) < 0 & \quad \alpha = 4, 5, 6 \end{aligned} \quad (31)$$

thus

$$p_\alpha^* = p_{\alpha+3}; \quad \xi_\alpha^* = \xi_{\alpha+3} \quad (\alpha = 1, 2, 3) \quad (32)$$

where * indicates a complex conjugation.

So far, p and \mathbf{A} can be derived upon solving the eigenvalue problem Eq. (28). There are three useful matrices, which will be mentioned in next section

$$\mathbf{Q}_{js} = i \sum_{\alpha=1}^6 \pm A_{j\alpha} A_{s\alpha} = 2i \sum_{\alpha=1}^3 A_{j\alpha} A_{s\alpha} \quad (33)$$

$$\mathbf{B}_{js} = i \sum_{\alpha=1}^6 \pm L_{j\alpha} L_{s\alpha} = 2i \sum_{\alpha=1}^3 L_{j\alpha} L_{s\alpha} \quad (34)$$

$$\mathbf{S}_{js} = i \sum_{\alpha=1}^6 \pm A_{j\alpha} L_{s\alpha} = i \left(\sum_{\alpha=1}^3 A_{j\alpha} L_{s\alpha} - \delta_{js} \right) \quad (35)$$

where "+" are used for $\alpha = 1, 2, 3$ and "-" are used for $\alpha = 4, 5, 6$.

For fixed C_{ijkl} and \mathbf{x} , the values of p_α and ξ_α are dependent on the choice of \mathbf{m} and \mathbf{n} ; however, \mathbf{Q} , \mathbf{B} and \mathbf{S} only depend on \mathbf{t} !

By the way, matrix \mathbf{Q} is intimately connected to the Green's function, as the orientation part

$$G_{ij}(\mathbf{x} - \mathbf{x}') = -\frac{Q_{ij}}{4\pi|\mathbf{x} - \mathbf{x}'|} \quad (36)$$

5.2 Solve for D

Following equation is an admissible solution to the elasticity equilibrium problem,

$$u_k = \frac{1}{2\pi i} \sum_{\alpha=1}^6 D_\alpha A_{k\alpha} \ln(\mathbf{m} \cdot \mathbf{x} + p_\alpha \mathbf{n} \cdot \mathbf{x}) \quad (37)$$

We can make a cut extending from $\mathbf{x} = 0$ to $\mathbf{m} \cdot \mathbf{x} \rightarrow \infty$ along \mathbf{m} direction. Our convention is such that for $\mathbf{m} \cdot \mathbf{x} > 0$,

$$\ln(\mathbf{m} \cdot \mathbf{x} + p_\alpha \mathbf{n} \cdot \mathbf{x}) \rightarrow \ln(\mathbf{m} \cdot \mathbf{x}) \pm i0 \quad \text{as } \mathbf{n} \cdot \mathbf{x} \rightarrow 0^+ \quad (38)$$

$$\rightarrow \ln(\mathbf{m} \cdot \mathbf{x}) \pm i2\pi \quad \text{as } \mathbf{n} \cdot \mathbf{x} \rightarrow 0^- \quad (39)$$

The discontinuity across the cut in u_i is given by

$$\Delta u_i = u_i(\mathbf{m} \cdot \mathbf{x} > 0; \mathbf{n} \cdot \mathbf{x} = 0^-) - u_i(\mathbf{m} \cdot \mathbf{x} > 0; \mathbf{n} \cdot \mathbf{x} = 0^+) \quad (40)$$

$$= \sum_{\alpha=1}^6 \pm A_{i\alpha} D_\alpha = b_i \quad (41)$$

Here we see that the choice of $f(\cdot) = \ln(\cdot)$ in Eq. (37) is important for the displacement jump condition for a dislocation to be satisfied. Hence the solution for D_α is

$$D_\alpha = \pm L_{s\alpha} b_s \quad (42)$$

where, the upper(lower) signs are used for $\alpha = 1, 2, 3$ (4, 5, 6).

Hence, the displacement field solution for a pure dislocation is

$$u_k = \frac{1}{2\pi i} \sum_{\alpha=1}^6 \pm A_{k\alpha} L_{s\alpha} b_s \ln(\mathbf{m} \cdot \mathbf{x} + p_\alpha \mathbf{n} \cdot \mathbf{x}) \quad (43)$$

6 Stress Field of Infinite Straight Line Dislocation

The stress field of an infinite straight dislocation line along direction \mathbf{t} with Burgers vector \mathbf{b} can be explicitly expressed in terms of the matrices \mathbf{Q} , \mathbf{S} , \mathbf{B} , which can be evaluated by either Stroh/Matrix formalism or Integral formalism. The stress field can be expressed in several different but equivalent forms.

6.1 In terms of angular stress factor Σ_{mn}

Given the dislocation line orientation \mathbf{t} , we can always find two unit vectors \mathbf{m} and \mathbf{n} , such that \mathbf{m} - \mathbf{n} - \mathbf{t} form a right-handed coordinate system. Obviously, the stress field at any point \mathbf{x} does not change if we move point \mathbf{x} along direction \mathbf{t} . Therefore, we can require vector \mathbf{x} to be parallel to vector \mathbf{m} without any

loss of generality, i.e. $\mathbf{x} = |\mathbf{x}|\mathbf{m}$. The stress field will be inversely proportional to the distance $|\mathbf{x}|$ and the proportional constant is called the angular stress factor Σ .

$$\sigma_{mn}^{\infty}(\mathbf{x} = |\mathbf{x}|\mathbf{m}) = \frac{1}{|\mathbf{x}|} \Sigma_{mn}(\mathbf{m}; \mathbf{t}, \mathbf{b}) \quad (44)$$

$$\Sigma_{mn} = \frac{1}{2\pi} C_{mni p} b_s \{ -m_p S_{is} + n_p (nn)_{ik}^{-1} [B_{ks} + (nm)_{kr} S_{rs}] \}$$

6.2 In terms of Willis–Steeds formula

Through the Generalized Hooke's law, the stress field can be expressed in terms of the displacement gradient, which is expressed in terms of matrices Q and S through the Willis-Steeds formula

$$\sigma_{ij} = C_{ijkl} \frac{\partial u_k}{\partial x_l} \quad (45)$$

$$\frac{\partial u_m}{\partial x_s} = \frac{1}{2\pi h} \epsilon_{j s n} b_i C_{ijkl} t_n \{ -m_l Q_{mk} + n_l [(nn)^{-1} \cdot (nm) \cdot Q]_{mk} + n_l [(nn)^{-1} \cdot S]_{mk} \}$$

Again, we require the field point \mathbf{x} to be parallel to vector \mathbf{m} without any loss of generality, i.e. $\mathbf{x} = |\mathbf{x}|\mathbf{m}$. Define $h = |\mathbf{x}|$.

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